Bisphenol B 77-40-7 | DTXSID4022442

Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (75	Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: 140 °C

Global applicability domain: Inside

Local applicability domain index: 9.01e-01

Confidence level: 6.49e-01

Nearest Neighbors from the Training Set

Image not found

Bisphenol B Measured: 121 Predicted: 140 Image not found

phenol, 4,4'-butylidenebis-

Measured: 137 Predicted: 142

Image not found

Bisphenol A
Measured: 153

Predicted: 144

Image not found

meso-Hexestrol Measured: 187 Predicted: 157 Image not found

4,4'-Propane-1,1-diyldiphenol

Measured: 132 Predicted: 133